LA-UR- 04-0552

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Submitted to: XXI Int. Conf of Theoretical & Applied Mechanics

Los Alamos
NATIONAL LABORATORY

ASSESSING DIFFERENT SELF-CONSISTENT APPROXIMATIONS BY COMPARISON WITH FULL-FIELD SIMULATIONS IN VISCOPLASTIC POLYCRYSTALS

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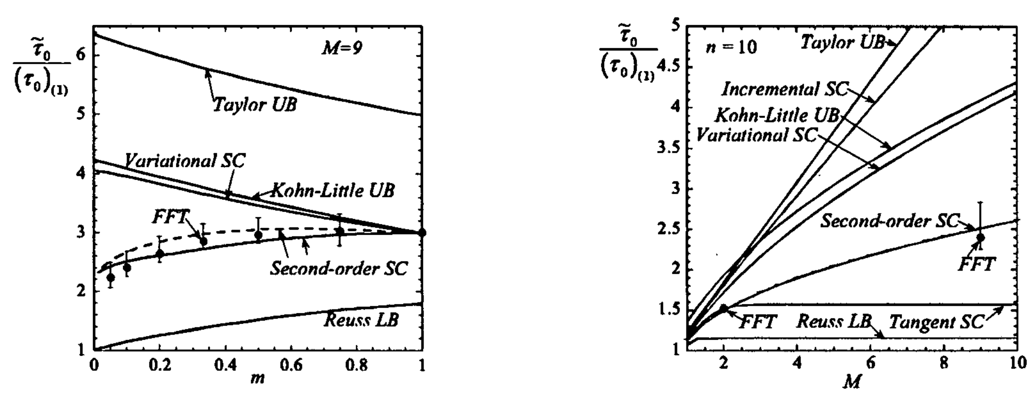
Summary In this work we compare full-field numerical simulations for the effective behavior and the statistical field fluctuations in 2-D and 3-D viscoplastic polycrystals with various estimates of the self-consistent (SC) type. For linear systems, the above comparison demonstrates the accuracy of the standard SC approximation. On the other hand, of the various non-linear self-consistent formulations, the recent 'second-order' method, based on a linearization that takes into account the second-order moments of the mechanical fields, gives the best overall agreement with the full-field simulations.

INTRODUCTION

Because most metals and minerals appear in polycrystalline form, the computation of the *effective* response of polycrystalline aggregates starting from the *properties* of their constituent single-crystal grains and the polycrystal's *microstructure* is a fundamental problem in materials science. For non-linear materials, several self-consistent (SC) models, such as the 'incremental' method of Hill [1], the 'tangent' procedure of Molinari *et al.* [2] and the 'affine' method of Masson *et al.* [3] are available. While these various approximations generally provide improvements on the Taylor and Reuss bounds, and reduce to the linear self-consistent estimate for linearly viscous behavior, they give widely diverging predictions for low rate-sensitivity materials. Alternative extensions of the SC estimates for viscoplastic polycrystals have been proposed recently making use of rigorous nonlinear homogenization methods. More specifically, these novel SC estimates are based on the use of 'variational' *linear comparison* methods, which express the effective potential of the nonlinear viscoplastic polycrystal in terms of that of a *linearly viscous* polycrystal [4] with properties that are determined from suitably designed variational principles. The most recent of these variational formulations is the 'second-order' method [5], which makes use of the SC approximation for a linear *thermoelastic* polycrystal to generate more accurate SC estimates for viscoplastic polycrystals that take into account the second order moments of the mechanical fields inside the constituent grains. On the other hand, the dramatic increases in computational power of recent years have begun to make possible full-field simulations of polycrystalline samples. Recently, a technique based on the use of Fast Fourier Transform (FFT) has been introduced by Moulinec and Suquet [6] and applications of the method have been given recently for polycrystals [7]. The aforementioned uncertainties associated with the various self-consistent schemes and the availability of powerful full-field numerical simulations suggest the computation of *ensemble averages* [8] of the later to verify the accuracy of the former.

RESULTS

2-D polycrystals



(a) (b)

Figure 1. Comparison of the 'second-order' SC estimates with the FFT simulation results, and the Taylor, Kohn-Little and Reuss bounds for the effective viscosity $\tilde{\tau}_0$: (*a*) as functions of the strain-rate sensitivity m for $M = (\tau_0)_{(2)}/(\tau_0)_{(1)} = 9$; (*b*) as functions of the grain anisotropy M for $n = 1/m = 10$. Also shown in (*a*) and (*b*) are the 'variational' SC estimates, and in (*b*) the 'incremental' and 'tangent' SC estimates.

We show here results for a special class of model polycrystals, consisting of columnar orthorhombic grains with random in-plane orientations. When such polycrystals are loaded in antiplane strain, only two slip systems (with flow stresses $(\tau_0)_{(1)}$ and $(\tau_0)_{(2)}$, respectively) can be activated and a 2-D boundary value problem is thus defined. This special class of 2-D polycrystals has received considerable attention in the literature in recent years, due to the fact that the effective stress is known to have an exact solution, $\tilde{\tau}_0 = \sqrt{(\tau_0)_{(1)}(\tau_0)_{(2)}}$, when the behavior of the single-crystals is linear. For more general power-law polycrystals, the exact result is not known, but an upper bound that is sharper than the classical Taylor bound is available [9]. In Fig. 1, different SC estimates for the effective viscosity $\tilde{\tau}_0$ are shown and compared with the FFT simulation results. Note that the 'error' bars for the FFT results correspond to the maximum and minimum values of $\tilde{\tau}_0$ over all the configurations in the ensemble. Figure 1(a) shows results for $\tilde{\tau}_0$ plotted as functions of the strain-rate sensitivity $m = 1/n$, for a fixed value of the grain anisotropy ($M = (\tau_0)_{(2)}/(\tau_0)_{(1)} = 9$). Figure 1($b$) shows results for $\tilde{\tau}_0$ as functions of the grain anisotropy M, for a fixed value of the nonlinearity ($n = 1/m = 10$). The results shown include the Taylor, Reuss and Kohn-Little bounds, the 'incremental' [1], 'tangent' [2] and 'variational' [4] SC estimates, as well as two slightly different versions of the 'second-order' [5] estimates (continuous and dashed lines). The main observations from these figures are: (i) all the various types of SC estimates satisfy the bounds, except the 'incremental' which violates the Kohn-Little bound, and (ii) the 'second-order' estimate appears to be the *only one* that is consistent with the FFT simulations, for values of $m = 1/n$ different from 1 (the linear case).

FCC polycrystals

Table 1 shows bounds, SC and FFT estimates for the effective flow stress and suitably normalized measures of the *overall standard deviation (SD)* associated with the stress and strain-rate fields (see [10] for details), for a random, non-linear ($n = 10$) FCC polycrystal deformed in uniaxial tension. As for the 2-D case, the 'second-order' SC estimates appear to give the best overall agreement with the FFT results.

model	$\tilde{\sigma}_0/\tau_0$	$\mathrm{SD}(\sigma_e)/\bar{\sigma}_e$	$\mathrm{SD}(\epsilon_e)/\bar{\epsilon}_e$
Taylor	2.905	0.568	0.
Reuss	2.201	0.	0.825
incremental	2.880	0.752	0.185
affine	2.741	0.576	0.752
tangent	2.617	0.349	0.947
variational	2.811	0.696	0.188
second-order	2.540	0.413	0.878
FFT	2.614	0.480	0.586

Table 1. Taylor, Reuss, different self-consistent, and FFT estimates of the effective flow stress and the overall field SD's for a non-linear, isotropic FCC polycrystal ($n = 10$).

CONCLUSIONS

Among the various nonlinear extensions of the self-consistent approximation, the 'second-order' variational method, gives the best overall agreement with the effective properties and field fluctuations obtained by means of FFT full-field simulations, for 2-D and 3-D polycrystals.

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